REMARKS

Claims 1-90 were pending. No claim has been allowed. By this amendment, claims 1-3, 14, 15, 19, 20, 37-72 and 74-78 have been amended. Claims 79-90 have been cancelled to advance the prosecution. Typographical errors have been corrected in claims 1, 76, and 78. The specification has also been amended to correct typographical errors. No new matter has been added. A marked-up version of the changes being made by the current amendment is attached.

I. Information Disclosure Statement

The Examiner states that the information disclosure statement filed March 20, 2000, does not comply with 37 CFR 1.98(a)(2). The applicant respectfully directs the Examiner to 37 CFR 1.98(d)(1), which states that "a copy of any patent, publication, pending U.S. application or other information, as specificed in paragraph (a) of this section, listed in an information disclosure state is required to be provided even if the patent, publication, pending U.S. application or other information was submitted to, or cited by, the Office in an earlier application, unless: (t)he earlier application is properly identified in the information disclosure statement and is relied on for an earlier effective filing date under 35 U.S.C. 120."

This present application is a continuation-in-part of U.S. application serial no. 09/174,856 filed on October 19, 1998, and thus relies on the filing date of the earlier application under 35 U.S.C. §120. This information can be found in the information disclosure statement filed March 20, 2000 and with the filed patent application. Copies of references "AE" – "BK" were submitted with U.S. application serial no. 09/174,856. Under 37 CFR 1.98(d)(1), no copies of these references were required in this application. However, to facilitate prosecution, copies of these references will be submitted in a supplemental information disclosure statement.

II. Section 112 Rejections

Claims 37-72, 74, 75, 77, and 78 were rejected as allegedly being indefinite because the Examiner found that it was unclear whether a computer program per se or a computer program

product on a computer-readable medium was claimed. The applicant submits that each of claims 37, 55, 66, and 72 is an independent claim directed to a computer program product on a computer-readable medium, and notes that each of the claims in question has been amended to clarify that it is the product, and not merely the program, that is the subject of the claims.

Claims 37-72 and 74-76 were rejected as allegedly lacking antecedent basis. Claims 37, 55, 66, and 72 have been amended to recite that it is "the computer program product" that comprises the instructions recited in the body of each claim. Dependent claims 38-54, 56-65, and 67-71 have been amended to refer back to the computer program product recited in a previous claim. Claims 74, 75, and 76 have also been amended to correct the claims' dependency. Claims 74 and 75 are dependent claims based on claim 73. Claim 76 is a dependent claim based on claim 37.

III. Section 101 Rejections

Claims 37-72, 74-75, and 77-78 were rejected under 35 U.S.C. § 101 as non-statutory subject matter. The applicant submits that the subject matter recited in each of the aforementioned claims, a computer program product on a computer-readable medium, is patentable subject matter under 35 U.S.C. § 101. "When functional descriptive material is recorded on some computer-readable medium it becomes structurally and functionally interrelated to the medium and will be statutory in most cases. . . . 'Functional descriptive material' consists of data structures and computer programs which impart functionality when encoded on a computer-readable medium." MPEP § 2106 IV.B.1. "If a claim defines a useful machine or manufacture by identifying the physical structure of a machine or manufacture in terms of its . . . hardware and software combination, it defines a statutory product. . . . A claim limited to a machine or manufacture, which has a practical application in the technological arts, is statutory." MPEP § 2106 IV.B.2(a). Finally, if a machine produces "a useful, concrete and tangible result" it is more than just a non-statutory abstract idea. *See State Street Bank and Trust Co. v. Signature Financial Group Inc.*, 149 F.3d 1368, 1373 (Fed. Cir. 1998).

Independent claims 37, 55, 66, and 72 recite computer program products that cause a programmable processor to perform a series of actions with the useful, concrete, and tangible

result of generating a representation of a library design for a combinatorial library of materials, with practical application in the field of materials science. The product is therefore functional. Claims 38-54, 56-65, 67-71, 74-75, and 77-78 all depend from the above independent claims. Accordingly, the applicant submits claims 37-72, 74-75, and 77-78 all recite statutory subject matter.

IV. Section 103 Rejections

Claims 1-90 were rejected under 35 U.S.C. § 103(a) as allegedly being unpatentable over U.S. Patent No. 5,930,154 ("Thalhammer-Reyero") in view of U.S. Patent No. 6,044,212 ("Flavin"). The applicant respectfully disagrees.

Neither of the references that the Examiner relies on discloses or suggests any method of generating a library design, much less a method that generates the representation of such a design that is recited in claim 1. The Examiner states that Flavin discloses the use of automated technology in chemical process research and development, but recognizes that Flavin does not teach receiving an input defining a mapping that, in turn, defines a distribution pattern for assigning a component to cells in an arrangement of cells, as claim 1 requires. Instead, the Examiner points to Thalhammer-Reyero for that subject matter, asserting that reference discloses: (1) receiving an input defining a mapping; (2) defining a distribution pattern; (3) using a mapping to calculate a composition; and (4) generating a data file defining a design.

Thalhammer-Reyero discloses techniques for modeling chemical and biochemical processes. *See* Abstract (describing a system "providing an environment for development and deployment of visual models of complex systems organized in discrete time and space compartments"). But the passages cited by the Examiner do not disclose anything like the mappings defining a distribution pattern for assigning components to destination locations as recited in claim 1, or the use of such mappings to calculate material compositions, as the claim also requires.

The Examiner first cites column 4, lines 60-62 of Thalhammer-Reyero, which recite: "This information is mapped into the graphic knowledge structures represented by the different classes of schematic tools". The "information" referred in this passage is "experimentally

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obtained qualitative information, such as the identification of biological entities and processes involved, the knowledge about their localization within discrete physiological compartments in space and time, and about the relationships and qualitative interactions between those entities." Thalhammer-Reyero, column 4, lines 55-60. The applicant submits that this has nothing to do with receiving input defining a mapping that defines a distribution pattern for components to be used in preparing a library of materials, which is the subject of claim 1 of the present application.

The Examiner appears to recognize this, pointing next to column 17, lines 16-19 of Thalhammer-Reyero as allegedly disclosing "defining a distribution pattern". But that passage is to be equally off-point, reciting that "The scaled-valued variables, such as scaled-amount, have values within the 0.0 to 100.0 scale to normalize the diverse ranges of magnitudes involved in the system." According to Thalhammer-Reyero, these scaled-valued variables represent "the knowledge about the physiological steady-state conditions" being modelled or simulated. *See* column 17, lines 21-22. The values describe the characteristics of the biological systems that may be present in each reaction as a ratio of quantities of interacting or regulatory molecules. *See* column 16, lines 65-67.

Thalhammer-Reyero's values therefore merely reflect the contents of a modelled biological system. But claim 1 expressly recites that the distribution pattern includes a minimum and a maximum amount of the component to be assigned to any cell of the arrangement and a gradient to be applied between the minimum and maximum amounts of the component across the plurality of cells. The applicant submits that the cited passage does not disclose or suggest such a distribution pattern.

Next, the Examiner cites lines 12-30 of column 29 of Thalhammer-Reyero as allegedly disclosing the use of a mapping to calculate a composition. But, while this passage may disclose modeling the transfer of molecules between "compartments" in a bio-process, it neither discloses nor suggests calculating a composition of a material assigned to a particular destination location, as claim 1 requires, much less the calculation of such a composition using a mapping of the type recited in claim 1 – that is, a mapping that defines a distribution pattern including a gradient applied to a component across locations in a destination arrangement.

Nor does Thalhammer-Reyero disclose the generation of a data file or other representation of a library design, as amended claim 1 requires. For this, the Examiner cites

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column 41, line 67 of Thalhammer-Reyero, but that line merely recites that values for variables of interest in a simulation can be "archived to a text file". By contrast, claim 1 expressly recites that the library representation includes electronic data representing the sources, destinations and mapping. As noted above, Thalhammer-Reyero does not disclose or suggest the mapping recited in claim 1; the applicant submits that it necessarily cannot generate a representation that includes data representing such a mapping.

Thalhammer-Reyero and Flavin fail to disclose at least the previously discussed limitations of claim 1. The applicant therefore submits that no *prima facie* showing of obviousness has been made with respect to claim 1, which is therefore allowable over the combination. Claims 2-18 and 73-75 are dependent claims based directly or indirectly on claim 1, and are therefore allowable for at least the reasons discussed above in connection with claim 1.

Claim 9 is allowable over Thalhammer-Reyero and Flavin for at least the following additional reason. Claim 9, which is based on claim 1, exemplifies gradient types that can be input into the method and are included in the distribution pattern. The gradient types in claim 9 can be linear, logarithmic, exponential, polynomial or geometric progressions.

The Examiner points to column 30, lines 30-31 of the Thalhammer-Reyero reference for an example of a linear progression. But these lines do not discuss linear progression, or any type of gradient. Because neither Thalhammer-Reyero nor Flavin, alone or in combination, disclose or suggest this limitation of claim 9, that claim is allowable for this reason in addition to the reasons discussed above in the context of claim 1.

Claim 19 recites a similar computer-implemented method in which the mappings define a set of equations for calculating an amount of one or more components to be assigned to one or more cells in an arrangement. The equations are used to calculate the composition of a material to be assigned to the cells. The applicant submits that the cited references fail to disclose or suggest receiving an input that includes such a mapping.

The Examiner states that Thalhammer-Reyero describes data defining a set of equations, *see* column 5, lines 1-3, and using the equations to calculate a composition, *see* column 5, lines 11-15. However, those equations are not equations for calculating an amount of components to be assigned to cells in an arrangement, as claim 1 requires. Rather, the equations discussed in the cited passages define the behavior of a modelled system. *See* Thalhammer-Reyero, column

5, line 1. For example, Thalhammer-Reyero discloses that kinetic equations can be used to calculate a prediction of the translocation of proteins through compartments. *See* column 5, lines 10-15 and column 29, lines 12-30.

Because Thalhammer-Reyero and Flavin both fail to disclose at least the elements of receiving input defining equations and using those equations to assign quantities of components to cells in an arrangement, the applicant submits that no *prima facie* showing of obviousness has been made, and that claim 19 and dependent claims 20-29 are allowable over the combination of Thalhammer-Reyero and Flavin.

Like claims 1 and 19, claim 30 is an independent claim directed to a method for generating a library design for a combinatorial library of materials. The method of claim 30 includes defining sets of sources and destinations and defining mappings that define a composition for each of a plurality of materials assigned to a plurality of cells in the arrangement. As amended, the claim further recites receiving an input defining one or more parameters corresponding to process parameters to be applied to cells in the arrangement and defining parameter values for cells of the arrangement, and generating a representation of the library design that includes electronic data describing the source elements, the destination elements, the mappings and the parameters. The specification explains that parameters can include any external conditions selected for each of the reaction cells. *See* page 25, line 23.

As discussed above, neither Thalhammer-Reyero nor Flavin discloses or suggests mappings that define the composition of materials assigned to cells in an arrangement of cells. Moreover, neither reference discloses generating a representation of a library design that includes data representing such mappings, or that represents parameters as claim 30 recites.

The Examiner cites column 2, lines 2-3 of Thalhammer-Reyero for an example of parameter values. But Thalhammer-Reyero's parameters are associated with the biological system that is being modelled, and do not represent external process parameters that can be applied to members of a combinatorial library, as amended claim 30 requires. Thus, for example, Thalhammer-Reyero's parameters may relate to rates of conversion or rates of translocation. *See* column 4, line 35. The applicant submits that these parameters are not process parameters as recited in claim 30. Because neither reference discloses or suggests at

least these limitations of claim 30, the applicant submits that claim 30, and dependent claims 31-35, are allowable over Thalhammer-Reyero and Flavin.

Claim 36 is an independent claim reciting a method for preparing a combinatorial library of materials on a substrate. The method includes creating a library design by defining a set of design elements that includes one or more sources representing components to be used in preparing the combinatorial library, one or more destinations representing an arrangement of one or more cells, and one or more mappings defining a scheme for assigning components to cells of an arrangement and/or parameters corresponding to process parameters to be applied to cells in the arrangement. The method further includes generating a representation of a library design that includes data describing the sources, the destinations, the mappings and the parameters. The representation is used to cause an automated material handling apparatus to assemble the combinatorial library on a substrate.

As discussed above, neither Thalhammer-Reyero nor Flavin discloses or suggests generating a representation of a library design that includes data representing mappings assigning components to library members or process parameters to be applied to such library members. The applicant also submits that neither reference discloses or suggests using such a library design to prepare a combinatorial library of materials, as claim 36 also requires. Accordingly, claim 36 is allowable over these references.

Claim 37, 55, 66 and claim 72 are computer program product claims that include limitations analogous to those discussed above in the context of claims 1, 19, 30 and 36, respectively. The applicant therefore submits that each of these claims, as well as dependent claims 38-54, 56-65, 67-71, and 76-78, which are based directly or indirectly on these claims, are allowable for at least the reasons discussed above with respect to claims 1, 19, 30 and 36.

IV. Conclusion

The applicant submits that all claims are in condition for allowance and asks that all claims be allowed. Enclosed is a $110.00 check for the Petition for Extension of Time fee. Please apply any other charges or credits to Deposit Account No. 06-1050.

Respectfully submitted,

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Version with markings to show changes made

In the specification:

Paragraph beginning at page 22, line 32 has been amended as follows:

The use of subtypes provides the user additional flexibility in designing a library using equations. For example, a user may design a library for copolymerizing pairs of monomers, with the monomers being added at different times during the polymerization reaction. By defining two chemical subtypes – for example, "first monomer" and "second monomer" – under single chemical type "monomer", the user may define the total amount of combined monomer using one equation (e.g., [(mg) monomer = 0.2 Total Mass]), while defining the [ration] ratio of the first monomer to the second monomer using a second equation (e.g., [(mg) first monomer = 0.3 second monomer]).

Paragraph beginning at page 29, line 31 has been amended as follows:

A library of such materials can be a physical array of candidate materials, comprising a substrate and two or more different candidate materials, and preferably four or more different candidate materials at separate portions of the substrate, corresponding to library members. Each candidate material can consist essentially of two components (or source materials -- *e.g.*, a combination of sources A and B). Alternatively, additional components can be incorporated in the library design, resulting in libraries of diverse materials having compositions that are essentially ternary, quaternary or higher order. Such higher-order compositions can be designed to include the same components (*e.g.*, A, B and C) in each composition, but in varying amounts or ratios, or alternatively, to include different components (*e.g.*, A, B and C; A, B and D; A, B and E; A, B and F, etc.) in two or more of the compositions. In one preferred library, [the] there is a spatially addressable array of materials that comprises a substrate having a surface and nine or more materials having different compositions at nine or more discrete regions of the substrate surface, with each material-containing region consisting essentially of one material. The nine or more materials preferably comprising two or more common components of interest, A and B, with the amount of at least one of the common components, A, preferably varying incrementally and uniformly between the nine or more materials, such that the nine or more materials form a

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uniform compositional gradient with respect to component A. The gradient can be linear, exponential, *etc.*, as described above. The amount of one or more additional components (*e.g.*, component B) can also vary. Non-gradient applications are also considered, as explained above in connection with the various mappings. In a particularly preferred library, the array comprises eleven or more materials at eleven or more discrete regions of the substrate, and at least one of the materials comprises component A and an essential absence of component B.

In the claims:

Claims 79-90 have been cancelled without prejudice.

Claims 1-3, 14, 15, 19, 20, 30, and 37-72, and 74-78 have been amended as follows:

1. (Amended) A computer-implemented method for generating a library design for a combinatorial library of materials, comprising:

defining one or more sources and one or more destinations, each source being electronic data representing a component to be used in preparing the combinatorial library and each destination being electronic data representing an arrangement of cells;

receiving an input defining a first mapping, the first mapping being electronic data defining a distribution pattern for assigning a component to cells in the arrangement, the distribution pattern including a minimum and a maximum amount of the component to be assigned to any cell of the arrangement and a gradient to be applied between the minimum and maximum amounts of the component across the plurality of cells;

using the first mapping to calculate a composition of one or more materials assigned to one or more of the cells; and

generating a [data file defining] representation of the library design, the [data file] representation comprising electronic data representing the sources, the destinations and the mapping.

2. (Amended) The method of claim 1, further comprising:

displaying a visual representation of the library design, the visual representation graphically describing the composition of one or more materials assigned to one or more of the

cells.

3. (Amended) The method of claim 1, wherein the [data file] representation comprises electronic data representing one or more sets of properties, each set of properties being associated with one of the sources, the destinations or the mapping.

14. (Amended) The method of claim 1, further comprising generating a modified library design by:

receiving an input redefining a source, a destination or a mapping;

recalculating the composition of one or more materials assigned to one or more of the cells; and

generating a [data file defining] representation of the modified library design.

15. (Amended) The method of claim 1, further comprising:

receiving an input defining one or more parameters, each parameter being electronic data corresponding to a process parameter to be applied to one or more cells of the arrangement and defining a parameter value for the one or more cells of the arrangement, the parameter value varying between a minimum and a maximum amount; and

wherein the [data file] representation further comprises electronic data representing the one or more parameters.

19. (Amended) A computer-implemented method for generating a library design for a combinatorial library of materials, comprising:

defining a set of one or more sources and one or more destinations, each source being electronic data representing a component to be used in preparing the combinatorial library and each destination being electronic data representing an arrangement of cells;

receiving an input defining a set of first mappings, the first mappings being electronic data defining a set of equations for calculating an amount of one or more components to be assigned to one or more cells in an arrangement;

using the set of equations to calculate a composition of a material assigned to one or more of the cells; and

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generating a [data file defining] representation of the library design, the [data file] representation comprising electronic data representing the sources, the destinations and the mappings.

20. (Amended) The method of claim 19, further comprising:

displaying a visual representation of the library design, the visual representation graphically describing the composition of one or more materials assigned to one or more of the cells.

30. (Amended) A computer-implemented method for generating a library design for a combinatorial library of materials, comprising:

defining a set of one or more sources and one or more destinations, each source being electronic data representing a component to be used in preparing the combinatorial library and each destination being electronic data representing an arrangement of cells;

defining a plurality of mappings, the mappings in the aggregate defining a composition for each of a plurality of materials assigned to a plurality of cells in the arrangement;

receiving an input defining one or more parameters, each parameter being electronic data corresponding to a process parameter to be applied to one or more cells of the arrangement and defining a parameter value for the one or more cells of the arrangement, the parameter value varying between a minimum and a maximum amount; and

generating a [data file defining] representation of the library design, the [data file] representation comprising electronic data describing the source elements, the destination elements, the mappings and the parameters.

36. (Amended) A computer-implemented method for preparing a combinatorial library of materials on a substrate, the method comprising:

creating a library design by defining a set of design elements, the set of design elements including one or more sources representing components to be used in preparing the combinatorial library, one or more destinations, each destination comprising an arrangement of one or more cells, and one or more elements selected from the group consisting of a mapping defining a scheme for assigning one or more amounts of a component to one or more cells of an

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arrangement and a parameter corresponding to a process parameter to be applied to one or more cells of the arrangement, the parameter defining a parameter value for the one or more cells of the arrangement, the parameter value varying between a minimum and a maximum amount;

generating a [data file defining] representation of a library design, the representation[data file]comprising electronic data describing the sources, the destinations, the mappings and the parameters; and

using the representation[data file] to cause an automated material handling apparatus to assemble the combinatorial library on a substrate.

37. (Amended) A computer program product on a computer-readable medium for generating a library design for a combinatorial library of materials, the computer program product comprising instructions operable to cause a programmable processor to:

receive an input defining one or more sources and one or more destinations, each source being electronic data representing a component to be used in preparing the combinatorial library and each destination being electronic data representing an arrangement of cells;

receive an input defining a first mapping, the first mapping being electronic data defining a distribution pattern for assigning a component to cells in the arrangement, the distribution pattern including a minimum and a maximum amount of the component to be assigned to any cell of the arrangement and a gradient to be applied between the minimum and maximum amounts of the component across the plurality of cells;

use the first mapping to calculate a composition of one or materials assigned to one or more of the cells; and

generate a [data file defining] representation of the library design, the [data file] representation comprising electronic data representing the sources, the destinations and the mapping.

38. (Amended) The computer program product of claim 37, further comprising instructions operable to cause a programmable processor to:

display a visual representation of the library design, the visual representation graphically describing the composition of one or more materials assigned to one or more of the cells.

39. (Amended) The computer program product of claim 37, wherein the [data file] representation comprises electronic data representing one or more sets of properties, each set of properties being associated with one of the sources, the destinations or the mapping.

40. (Amended) The computer program product of claim 37, wherein the input defining the sources and destinations comprises an input from a graphical input device.

41. (Amended) The computer program product of claim 37, wherein the input defining a first mapping comprises a selection from a set of available mapping types, the set of available mapping types comprising a one to one mapping of a component from a source to a cell in the arrangement and a one to many mapping of a component from a source to a plurality of cells in the arrangement.

42. (Amended) The computer program product of claim 41, wherein the set of available mapping types further comprises a many to many mapping of a plurality of components from a plurality of sources to a plurality of cells in the arrangement.

43. (Amended) The computer program product of claim 42, wherein the set of available mapping types further comprises a many to one mapping of a plurality of components from a plurality of sources to a cell in the arrangement.

44. (Amended) The computer program product of claim 40, wherein the set of available mapping types further comprises a set of one or more user-defined equations.

45. (Amended) The computer program product of claim 37, wherein the gradient is selected from the group consisting of linear, logarithmic, exponential, polynomial and geometric progression.

46. (Amended) The computer program product of claim 39, wherein the set of properties associated with the mapping comprises a source name, a source geometry, a destination name, a destination geometry, a gradient type, and a set of gradient parameters defining the gradient.

47. (Amended) The computer program product of claim 37, further comprising instructions

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operable to cause a programmable processor to:

receive an input defining a second mapping, the second mapping being electronic data defining a second distribution pattern for distributing a second component to cells in the arrangement; and

use the first and second mappings to calculate a composition of one or more materials assigned to one or more of the cells.

48. (Amended) The computer program product of claim 47, wherein the second distribution pattern for assigning a second component includes electronic data identifying a fixed amount of the second component to be assigned to one or more cells in the arrangement.

49. (Amended) The computer program product of claim 48, wherein the second distribution pattern for assigning a second component includes electronic data identifying a minimum and a maximum amount of the second component to be assigned to any of the cells of the arrangement and a second gradient to be applied between the minimum and maximum amounts of the second component across the cells.

50. (Amended) The computer program product of claim 37, further comprising instructions operable to cause a programmable processor to generate a modified library design by receiving an input redefining a source, a destination or a mapping; recalculating the composition of one or more materials assigned to one or more of the cells; and generating a [data file] representation defining the modified library design.

51. (Amended) The computer program product of claim 37, further comprising instructions operable to cause a programmable processor to:

receive an input defining one or more parameters, each parameter being electronic data corresponding to a process parameter to be applied to one or more cells of the arrangement and defining a parameter value for the one or more cells of the arrangement, the parameter value varying between a minimum and a maximum amount; and

wherein the [data file] representation further comprises electronic data representing the one or more parameters.

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52. (Amended) The computer program product of claim 37, wherein the arrangement comprises two or more cells.

53. (Amended) The computer program product of claim 37, wherein the arrangement comprises ten or more cells.

54. (Amended) The computer program product of claim 37, wherein the arrangement comprises about ninety-six or more cells.

55. (Amended) A computer program product on a computer-readable medium for generating a library design for a combinatorial library of materials, the computer program product comprising instructions operable to cause a programmable processor to:

receive an input defining a set of one or more sources and one or more destinations, each source being electronic data representing a component to be used in preparing the combinatorial library and each destination being electronic data representing an arrangement of cells;

receive an input defining a set of first mappings, the first mappings being electronic data defining a set of equations for calculating an amount of one or more components to be assigned to one or more cells in an arrangement;

use the set of equations to calculate a composition of a material assigned to one or more of the cells; and

generate a [data file defining] representation of the library design, the [data file] representation comprising electronic data representing the sources, the destinations and the mappings.

56. (Amended) The computer program product of claim 55, further comprising instructions operable to:

display a visual representation of the library design, the visual representation graphically describing the composition of one or more materials assigned to one or more of the cells.

57. (Amended) The computer program product of claim 55, wherein the component to be assigned to a cell in the arrangement is determined by the location of the cell within the arrangement.

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58. (Amended) The computer program product of claim 57, wherein the composition of a material is determined using a subset of the set of equations, the subset of equations being determined by the location of the cell within the arrangement.

59. (Amended) The computer program product of claim 55, further comprising instructions operable to:

generate an error indicator signal if the number of equations in the set of equations is not equal to the number of sources in the set of sources.

60. (Amended) The computer program product of claim 55, wherein at least one of the set of equations is selected from the group consisting of:

a ratio equation defining an amount of a component to be assigned to a cell as a function of an amount of another component to be assigned to the cell;

a volume equation defining an amount of a component to be assigned to a cell as a function of a total volume of a plurality of components to be assigned to the cell; and

a mass equation defining an amount of a component to be assigned to a cell as a function of a total mass of a plurality of components to be assigned to the cell.

61. (Amended) The computer program product of claim 55, wherein the set of equations comprises a gradient equation defining an amount of a component to be assigned to each of a plurality of cells according to a gradient.

62. (Amended) The computer program product of claim 55, wherein each of the set of equations is assigned to one or more cells of the arrangement according to the location of the cells within the arrangement.

63. (Amended) The computer program product of claim 55, wherein the instructions operable to cause a programmable processor to use the set of equations to calculate a composition of a material assigned to one or more of the cells comprise instructions simultaneously to solve a set of interdependent equations.

64. (Amended) The computer program product of claim 63, wherein the instructions

simultaneously to solve the set of interdependent equations further comprise instructions to use a matrix inversion technique to solve the set of equations.

65. (Amended) The computer program product of claim 55, further comprising instructions operable to:

receive an input defining a second mapping, the second mapping being electronic data defining a distribution pattern for distributing a component to cells in the arrangement, the distribution pattern including a minimum and a maximum amount of the component to be assigned to any cell of the cells of the arrangement and a gradient to be applied between the minimum and maximum amounts of the component across the plurality of cells; and

use the first set of mappings and the second mapping to calculate a composition of a material assigned to one or more of the cells.

66. (Amended) A computer program product on a computer-readable medium for generating a library design for a combinatorial library of materials, the computer program product comprising instructions operable to cause a programmable processor to:

receive an input defining a set of one or more sources and one or more destinations, each source being electronic data representing a component to be used in preparing the combinatorial library and each destination being electronic data representing an arrangement of cells;

receive an input defining a plurality of mappings, the mappings in the aggregate defining a composition for each of a plurality of materials assigned to a plurality of cells in the arrangement;

receive an input defining one or more parameters, each parameter being electronic data corresponding to a process parameter to be applied to one or more cells of the arrangement and defining a parameter value for the one or more cells of the arrangement, the parameter value varying between a minimum and a maximum amount; and

generate a [data file defining] representation of the library design, the [data file] representation comprising electronic data describing the source elements, the destination elements, the mappings and the parameters.

67. (Amended) The computer program product of claim 66, wherein the parameter value is

defined to vary over time.

68. (Amended) The computer program product of claim 66, wherein the parameter value is defined to vary across two or more cells in the arrangement.

69. (Amended) The computer program product of claim 66, wherein the parameter value is defined to vary over time and across two or more cells in the arrangement.

70. (Amended) The computer program product of claim 66, wherein the parameter value varies according to a gradient selected from the group consisting of linear, logarithmic, exponential, polynomial and geometric progression.

71. (Amended) The computer program product of claim 66, wherein the parameter value corresponds to a process parameter selected from the group consisting of temperature, pressure, time, flow rate and stirring speed.

72. (Amended) A computer program product on a computer-readable medium for generating a library design for a combinatorial library of materials, the computer program product comprising instructions operable to cause a programmable processor to:

create a library design by defining a set of design elements, the set of design elements including one or more sources representing components to be used in preparing the combinatorial library, one or more destinations, each destination comprising an arrangement of one or more cells, and one or more elements selected from the group consisting of a mapping defining a scheme for assigning one or more amounts of a component to one or more cells of an arrangement and a parameter corresponding to a process parameter to be applied to one or more cells of the arrangement, the parameter defining a parameter value for the one or more cells of the arrangement, the parameter value varying between a minimum and a maximum amount;

generate a [data file]representation comprising electronic data describing the sources, the destinations, the mappings and the parameters; and

use the [data file]representation to cause an automated material handling apparatus to assemble the combinatorial library on a substrate.

74. (Amended) The method of claim 73, wherein:

at least one of the source properties is selected from the group consisting of molecular weight, equivalents, density and concentration.

75. (Amended) The method of claim 73, wherein:

at least one of the source properties is a type describing a class of chemicals to be used in generating the library design.

76. (Amended) The computer program product of claim 37, wherein:

each of the sources has an associated set of source properties describing the source; and

the instructions operable to cause a programmable processor to define the sources include instructions operable to cause a programmable processor to receive for each of the sources a set of values for one or more of the source properties associated with the source.

77. (Amended) The computer program product of claim 76, wherein:

at least one of the source properties is selected from the group consisting of molecular weight, equivalents, density and concentration.

78. (Amended) The computer program product of claim 76, wherein:

at least one of the source properties is a type describing a class of chemicals to be used in generating the library design.

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